

## Supporting Information

for

### **Controlling Hydrogen Release from Remaining-Intact Clathrate Hydrates by Electromagnetic Fields: Molecular Engineering via Microsecond Nonequilibrium Molecular-Dynamics**

Yogeshwaran Krishnan, Patricia Gomez Rosingana, Mohammad Reza Ghaani\* and Niall J. English\*

School of Chemical and Bioprocess Engineering, University College Dublin,  
Belfield, Dublin 4, Ireland

Correspondence: mohammad.ghaani@ucd.ie (M.R.G.); Tel.: +353-1-716-1758 (M.R.G.);  
niall.english@ucd.ie (N.J.E.); Tel.: +353-1-716-1646 (N.J.E.); Fax: +353-1-716-1177 (N.J.E.)

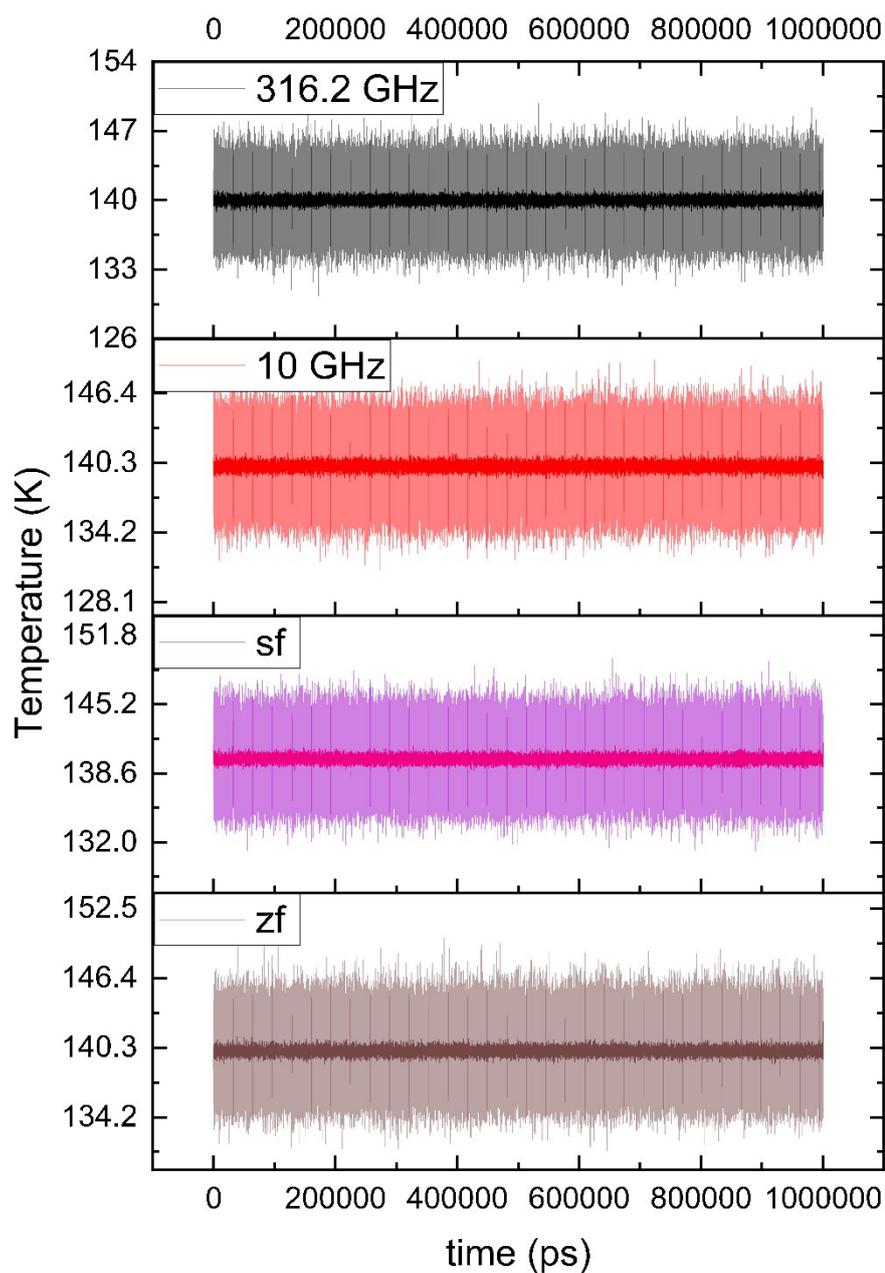


Figure S1. Temperature versus time of clathrate hydrates under the influence of a) zero field (zf), b) static field (sf), c) 10 GHz and d) 316.2 GHz

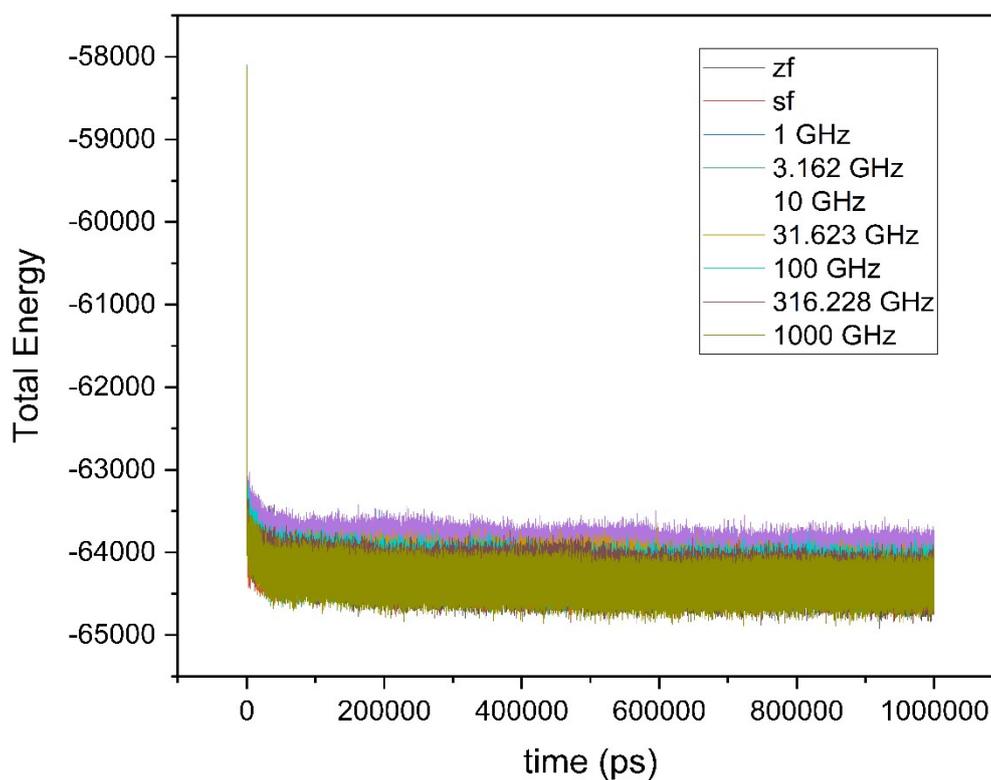


Figure S2. Total-system potential energy (kJ/mol) versus time of clathrate hydrates under the influence of .a) zero field (zf), b) static field (sf), c) 10 GHz and d) 1000 GHz

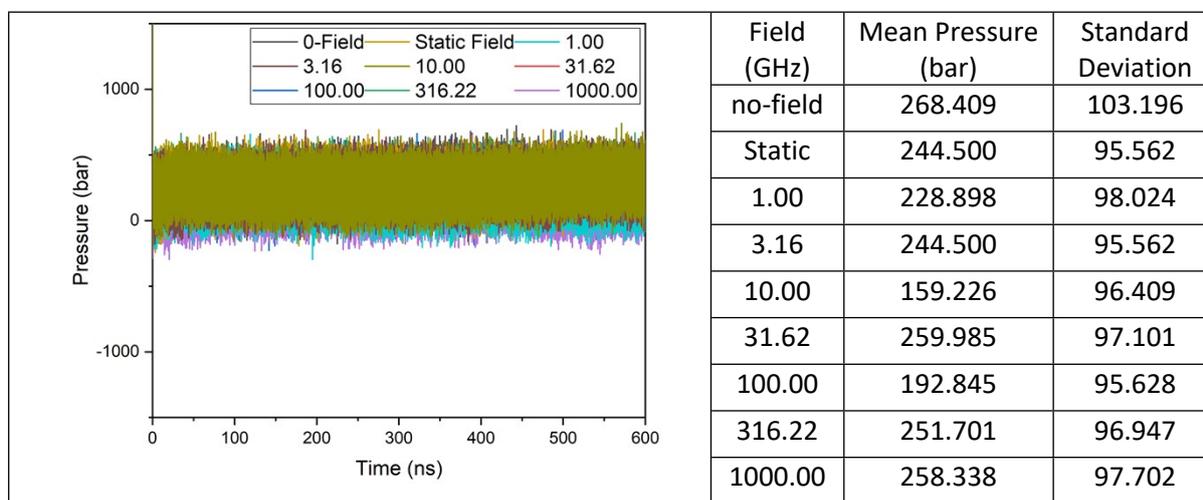


Figure S3. System Pressure (bar) versus time of clathrate hydrates under the influence of zero field, static field and 1 GHz to 1000 GHz.